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Fully Discrete Methods for the Nonlinear Schrödinger Equation

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Abstract—In this paper, we construct and analyze fully discrete methods for the nonlinear Schrödinger equation. These methods are based on a Galerkin-finite element formulation in space and use time stepping techniques which are modifications of implicit Runge-Kutta methods. The resulting schemes are both efficient and circumvent the well-known order reduction phenomenon affecting Runge-Kutta methods. Numerical experiments are also presented.

Keywords—Schrödinger equation, Higher order, Implicit Runge-Kutta method, L_2-convergence.

1. INTRODUCTION

Let Ω be a bounded domain in R^d, $d \geq 1$, with smooth boundary $\partial\Omega$, and let $0 < T < \infty$ be given. We consider the problem of approximating a complex-valued function $u(x,t)$ satisfying

$$\begin{aligned} u_t &= -iLu + f(x,t,u), && (x,t) \in \overline{\Omega} \times [0,T], \\ u &= 0, && (x,t) \in \partial\Omega \times [0,T], \\ u(x,0) &= u^0(x), && x \in \overline{\Omega}, \end{aligned} \tag{1.1}$$

where $-Lu = \sum_{j=1}^d \partial_{x_j}^2 u$ and u^0 is a given complex-valued function on $\overline{\Omega}$. The initial data u^0 and f are assumed to be such that (1.1) admits a solution sufficiently smooth to guarantee the convergence results to be presented below. For details about the physical significance and various properties of existence and uniqueness of the NLS equation, see [1–5].

In this work, we shall approximate the solution of (1.1) using a Galerkin-finite element type method for the spatial discretization, and implicit Runge-Kutta (IRK) methods for the time stepping. The IRK methods are modified by replacing the nonlinear term by an expression involving only previously known quantities. This approach, which basically consists of an extrapolation technique, has two advantages over the usual implementation: First, the scheme is implicit in the linear term and explicit in the nonlinear term; as a result, the linear systems that have to be solved at every time level involve fixed matrices. Second, by choosing the extrapolated values appropriately, the temporal rates of convergence can be shown to be those of the classical ones, i.e., those that are obtained for nonstiff problems, thus obviating the order reduction phenomenon that is known to occur in similar situations.

Concerning the classical implementation of IRK methods, O. Karakashian, G. Akrivis, and V. Dougalis established in [6] that the temporal errors decrease at the rate of at least $O(k^\sigma)$ in the case of the cubic Schrödinger equation (i.e., with $f(u) = i\lambda|u|^2 u$, $\lambda \in R \setminus \{0\}$). Here, $\sigma = \min\{p+3, \nu\}$ with p denoting the stage accuracy of the IRK method and ν the classical

Typeset by $\mathcal{A}_{\mathcal{M}}\mathcal{S}$-TEX accuracy (cf. [7]). This would indicate, although these estimates are not as of yet known to be sharp, that the convergence rates of the classical implementation are suboptimal. For instance, in the case of a q-stage Gauss-Legendre method, $\nu = 2q$ while $p = q$. Hence, for this class of methods, the rates would be suboptimal for $q \geq 4$.

The idea of using extrapolation for handling nonlinear terms efficiently is quite old. Relatively recently, G. Baker, V. Dougalis and O. Karakashian analyzed an extrapolation type multistep method for semilinear hyperbolic and parabolic equations [8]. In [9], Keeling constructed and analyzed extrapolation methods adapted to IRK methods in the context of semilinear and quasilinear parabolic problems. We follow his approach to approximate solutions of (1.1). The main difference here is the fact that the differential operator as well as the solution are complex valued.

The remainder of the paper is organized as follows. Section 2.1 is devoted to notation and preliminaries. In Section 2.2, the spatial discretization is introduced. In Section 2.3, the temporal discretization is introduced and the result of this paper is stated. In Section 3, we provide proofs of convergence at the optimal rates of the numerical schemes. In Section 4, we briefly consider the NLS equation with periodic B.C. Finally, in Section 5, computational results are presented.

2. FULLY DISCRETE METHODS

2.1. Notation and Preliminaries

For $1 \leq p \leq \infty$, $L^p = L^p(\Omega)$ will denote the Banach space of complex-valued measurable functions defined on Ω equipped with the norm $\|v\|_{L^p}$. (In the sequel, we use $\|\cdot\|$ instead of $\|\cdot\|_{L^2}$.)

For an integer $s \geq 0$ and $1 \leq p \leq \infty$, $W^{s,p}$ will denote the Banach space of complex-valued measurable functions which, together with their distributional derivatives of order up to s, are in L^p. In addition, let H_0^1 be the subspace of H^1 consisting of functions vanishing on $\partial\Omega$ in the sense of trace. We shall use the symbol H^s for $W^{s,2}$, and $\|\cdot\|_s$ instead of $\|\cdot\|_{s,2}$. Further, $\|\cdot\|_{s,\infty}$ represents the norm on $L^\infty([0,T], H^s)$.

Let L be extended to have domain $H^2 \cap H_0^1$. Then L is L_2-selfadjoint and for every nonnegative integer s, it is bounded from $H^{s+2} \cap H_0^1$ into H^s. Furthermore, introducing the solution operator T for the elliptic problem

$$\begin{aligned} Lv &= w, \qquad &&\text{in } \Omega, \\ v &= 0, \qquad &&\text{on } \partial\Omega, \end{aligned}$$

as $Tw \equiv v$, it is well known [10] that for every nonnegative integer s, T is bounded from H^s into $H^{s+2} \cap H_0^1$. Also, the solution operator is positive definite and self-adjoint on L^2.

2.2. The Spatial Discretization

In terms of the solution operator, (1.1) can be written as

$$\begin{aligned} \partial_t Tu &= -iu + Tf, \\ u(0) &= u^0. \end{aligned} \tag{2.1}$$

Let $\{S_h\}$ be a family of finite dimensional subspaces of H_0^1. We assume that a corresponding family of operators $\{T_h\}_{0<h<1}$ is given satisfying:

(i) $T_h : L^2 \to S_h$ is selfadjoint, positive semidefinite on L^2, and positive definite on S_h.
(ii) There is an integer $r \geq 2$ such that:

$$\|(T - T_h)v\| \leq Ch^s \|v\|_{s-2}, \qquad \forall v \in H^{s-2}, \quad 2 \leq s \leq r. \tag{2.2}$$

Now problem (2.1) has the following semidiscrete formulation. Find $u_h : [0,T] \to S_h$ such that

$$\begin{aligned} \partial_t T_h u_h &= -iu_h + T_h f_h, \\ u_h(0) &= u_h^0, \end{aligned} \tag{2.3}$$

where f_h represents f depending on u_h instead of u as indicated in (1.1) and $u_h^0 \in S_h$ is a suitable approximation to u^0. We shall assume that $S_h \subset L^\infty$ and

$$\|\chi\|_{L^\infty} \le Ch^{-d/2}\|\chi\|, \qquad \forall \chi \in S_h. \tag{2.4}$$

According to the properties described above, the restriction of T_h to S_h is invertible and its inverse is denoted by L_h. Then L_h satisfies the following properties:

$$(L_h v, v) \text{ is real for } v \in S_h \text{ and } (L_h v, v) \ge c\|v\|_1^2, \qquad \forall v \in S_h,$$

for some constant c independent of h.

Denoting the elliptic projection operator as $P_E = T_h L$, it follows from (2.2) that

$$\|(I - P_E)v\| \le ch^s\|v\|_s, \qquad \forall v \in H^s \cap H_0^1, \quad 2 \le s \le r. \tag{2.5}$$

Also, it can be shown that $L_h T_h = P_0$ is the orthogonal projection of L^2 onto S_h. Then, since $I - P_0$ is majorized by $I - P_E$ in L^2, it follows from (2.5) that

$$\|(I - P_0)v\| \le ch^s\|v\|_s, \qquad \forall v \in H^s \cap H_0^1, \quad 2 \le s \le r. \tag{2.6}$$

In addition to (2.5), with $w(t) = P_E u(t)$, we assume that

$$\sup_{0\le t\le T} \|u(t) - w(t)\|_{L^\infty} = r_0(h) \to 0, \qquad \text{as } h \to 0. \tag{2.7}$$

It can be shown (cf., e.g., [11]) that under reasonable assumptions there holds $r_0(h) \le ch^{r-d/2}$.

Now problem (2.3) takes the following form: Find $u_h : [0,T] \to S_h$ satisfying

$$\begin{aligned} \partial_t u_h &= -iL_h u_h + P_0 f_h, \\ u_h(0) &= u_h^0. \end{aligned} \tag{2.8}$$

In the present work, semidiscrete approximations are not analyzed. Instead, (2.8) serves only as a motivation for the construction of the fully discrete approximations.

2.3. The Temporal Discretizations

For $q \ge 1$ integer, a q-stage IRK method is characterized by a set of constants arranged in the following tableau form:

$$\begin{array}{ccc|c} a_{11} & \cdots & a_{1q} & \tau_1 \\ \vdots & & \vdots & \vdots \\ a_{q1} & \cdots & a_{qq} & \tau_q \\ \hline b_1 & \cdots & b_q & \end{array} .$$

It is convenient to make the following definitions:

$$A = (a_{ij})_{l\le i,\ j\le q}, \quad T = \operatorname*{diag}_{q\times q}\{\tau_i\}, \quad b^T = \langle b_1, b_2, \dots, b_q\rangle,$$
$$e^T = \langle 1, 1, \dots, 1\rangle \in R^q.$$

Given the initial value problem

$$\begin{aligned} y' &= f(t,y), \qquad 0 \le t \le T, \\ y(0) &= y_0, \end{aligned} \tag{2.9}$$

IRK methods can be applied to generate approximations y^n to $y(t^n)$ where $k = T/N$ is the temporal stepsize and $t^n = nk$, as follows: Let $y^0 = y_0$ and

$$y^{n+1} = y^n + k\sum_{j=1}^{q} b_j f\left(t^{n,j}, y^{n,j}\right), \tag{2.10}$$

where $t^{n,j} = t^n + \tau_j k$ and where the intermediate stages $y^{n,j}$ are given by the coupled system of equations

$$y^{n,j} = y^n + k\sum_{m=1}^{q} a_{jm} f(t^{n,m}, y^{n,m}), \qquad j = 1, 2, \dots, q. \tag{2.11}$$

To achieve the maximum order of accuracy for the temporal component of the error, we assume the following consistency relations

$$l!b^T A^{l-1} e = 1, \qquad 1 \le l \le \nu, \tag{2.12}$$

for some integer $\nu \ge 1$. To illuminate Condition (2.12), let (2.9) have $f(t,y) = -iy$ so that $y(t) = e^{-it}y_0$. Then from (2.10) and (2.11), $y^n = r(ik)^n y^0$ where $r(z)$ is the rational approximation to the exponential function e^{-z} given by

$$r(z) \equiv 1 - zb^T(I + zA)^{-1} e. \tag{2.13}$$

Expanding this expression shows that $r(z)$ is a ν^{th} order approximation to the exponential e^{-z} if and only if (2.12) holds.

Next, with regard to stability, assume that

$$|r(iy)| \le 1, \qquad y \ge 0. \tag{2.14}$$

Note that this condition is weaker than A-stability and is also weaker than the I-stability condition introduced in [12].

Note that the spectrum of A, $\sigma(A)$, consists of the negative reciprocals of the poles of $r(z)$. Hence, we shall assume that

$$\sigma(A) \subset \{z \in C \mid \operatorname{Re} z \ne 0\}. \tag{2.15}$$

We shall also assume that f satisfies the following local Lipschitz property: There exist constants $\rho, C(\rho, u)$ such that

$$\begin{gathered} |u(x,t) - v| \le \rho \to |f(x,t,u(x,t) - f(x,t,v)| \le C(\rho,u)\,|u(x,t) - v|, \\ \text{for all } (x,t) \in \Omega \times [0,T]. \end{gathered} \tag{2.16}$$

Returning to the temporal discretization of (2.8), let a q-stage IRK method of order $\nu \ge 1$ be given. We define constants $[\alpha_{j,m}]_{1\le j\le q}^{0\le m\le \nu-1}$ by

$$\sum_{m=0}^{\nu-1} \alpha_{j,m} m^l = (-1)^l\, l!\hat{e}_j^T A^l e, \qquad 1 \le j \le q, \quad 0 \le l \le \nu - 1, \tag{2.17}$$

with $(m^l\,|_{m=l=0}=1)$ and where $\hat{e}_j \in R^q$ denotes the j^{th} element of the canonical basis. Since the $\nu \times \nu$ Vandermonde matrix $(m^l)_{0\le m,\,l\le \nu-1}$ is nonsingular, the constants $\alpha_{j,m}$ are well-defined. Now suppose that approximations $[U_h^m]_{m=0}^n \subset S_h$ are given where $U_h^m \approx u^m = u(x,t^m)$. Define the extrapolation operators $\varepsilon^n : [L^2]^\nu \to [L^2]^q$ to have components

$$\varepsilon_j^n f_h \equiv \sum_{m=0}^{\nu-1} \alpha_{j,m} f\left(x, t^{n-m}, U_h^{n-m}\right), \qquad j=1,\ldots,q. \tag{2.18}$$

Also, define $\mathcal{L}_h : (S_h)^q \to (S_h)^q$ and $\mathcal{P}_0 : (L^2)^q \to (S_h)^q$ by

$$\mathcal{L}_h = \operatorname*{diag}_{q\times q}\{L_h\} \text{ and } \mathcal{P}_0 = \operatorname*{diag}_{q\times q}\{P_0\}.$$

Finally, let $U_h^{n+1} \cong u^{n+1}$ be given by what will thereafter be called the principal scheme

$$\begin{aligned} \mathcal{U}_h^n &= eU_h^n - ikA\mathcal{L}_h\mathcal{U}_h^n + kA\mathcal{P}_0\varepsilon^n f_h, \\ U_h^{n+1} &= U_h^n - ikb^T\mathcal{L}_h\mathcal{U}_h^n + kb^T\mathcal{P}_0\varepsilon^n f_h. \end{aligned} \tag{2.19}$$

Note that (2.19) is only partially patterned after (2.10) and (2.11), i.e., the intermediate stages $\mathcal{U}_h^n$ are not fully implicit, and extrapolation circumvents the solution of a nonlinear system of algebraic equations for each n.

Since the extrapolation for the principal scheme uses previously computed approximations, a starting procedure is required to generate $[U_h^n]_{n=0}^{\nu-1}$. We shall refer to this as the starting procedure. For $n=0$, we take as U_h^0 any element of S_h which is optimally close to u^0 in L^2, i.e.,

$$\left\|u^0 - U_h^0\right\| \le ch^r. \tag{2.20}$$

In particular, we shall work with $U_h^0 = P_0 u^0$.

Now, for $1 \le s \le \nu-1$, let the constants $[\alpha_{j,m}^{n,s}]_{0\le m\le s-1,\,1\le j\le q}^{0\le n\le s-1}$ be determined by

$$\sum_{m=0}^{s-1} \alpha_{j,m}^{n,s}(m-n)^l = l!\hat{e}_j^T A^l e, \qquad 1\le j\le q, \quad 0\le l\le s-1. \tag{2.21}$$

Let $U_h^{0,s} = U_h^0$, $s \ge 0$. Furthermore, for $s=1,\ldots,\nu-1$, $m=0,\ldots,s-1$ let $U_h^{m,s} \approx u^m$ be given by

$$\begin{aligned} \mathcal{U}_h^{n,s} &= eU_h^{n,s} - ikA\mathcal{L}_h\mathcal{U}_h^{n,s} + kA\mathcal{P}_0\varepsilon^{n,s} f_h, \\ U_h^{n+1,s} &= U_h^{n,s} - ikb^T\mathcal{L}_h\mathcal{U}_h^{n,s} + kb^T\mathcal{P}_0\varepsilon^{n,s} f_h, \end{aligned} \tag{2.22}$$

where the extrapolation operators $\varepsilon^{n,s} : [L^2]^s \to (L^2)^q$ have components

$$\begin{aligned} \varepsilon_j^{n,s} f_h &= \sum_{m=0}^{n} \alpha_{j,m}^{n,s} f\left(x, t^m, U_h^{m,s}\right) \\ &\quad + \sum_{m=n+1}^{s-1} \alpha_{j,m}^{n,s} f\left(x, t^m, U_h^{m,s-1}\right), \qquad 0\le n\le s-2, \\ \varepsilon_j^{n,s} f_h &= \sum_{m=0}^{s-1} \alpha_{j,m}^{n,s} f\left(x, t^m, U_h^{m,s}\right), \qquad n=s-1\le \nu-2. \end{aligned} \tag{2.23}$$

Note that both the principal and starting procedures are well-defined provided the operator $[I + ikA\mathcal{L}_h] : (S_h)^q \to (S_h)^q$ is invertible.

The error committed by the principal scheme (2.19) in the approximation of the solution of (1.1) will be shown to be of optimal order in the L^2-norm, i.e.,

$$\max_{\nu\le n\le N} \|U_h^n - u^n\| \le c(k^\nu + h^r), \tag{2.24}$$

where $u^n = u(\cdot, t^n)$. Concerning the starting scheme (2.22),(2.23), it can be shown that

$$\max_{0\le n\le \nu-1} \left\|U_h^{n,\nu-1} - u^n\right\| \le c(k^\nu + h^r). \tag{2.25}$$

The proof of this estimate is similar to the one that will be given concerning the principal scheme, so we omit it.

3. THE PRINCIPAL SCHEME

The following result establishes the invertibility of the operator $[I + ikA\mathcal{L}_h]$ together with a needed stability estimate.

LEMMA 3.1. *Assume that* (2.15) *holds. Then* $[I + ikA\mathcal{L}_h]$ *is invertible and*

$$\left\|(k\mathcal{L}_h)^{\theta} \left[I + ikA\mathcal{L}_h\right]^{-1} \chi\right\| \le c\|\chi\|, \qquad \forall \chi \in S_h, \quad 0 \le \theta \le 1. \tag{3.1}$$

PROOF. Let $S^{-1}\Lambda S$ be the Jordan decomposition of A, with Λ an upper triangular matrix, then $I + ikA\mathcal{L}_h = S^{-1}(I + ik\Lambda\mathcal{L}_h)\,S$. Let Λ_s be the $i_s \times i_s$ block of Λ corresponding to the eigenvalue λ_s, and consider the diagonal operator $\mathcal{L}_h^s = \operatorname{diag}\{L_h, L_h, \dots, L_h\}$ on $(S_h)^{i_s}$. We can show that $I + ikA\mathcal{L}_h$ is invertible in the following way. Assume that $\phi + ik\lambda_s L_h \phi = 0$. Then $(\phi,\phi) + ik\lambda_s(L_h\phi,\phi) = 0$ implies $\phi = 0$, since $(L_h\phi,\phi) > 0$ if $\phi \ne 0$ and $\operatorname{Re}\lambda_s \ne 0$. It follows that $I + ikA\mathcal{L}_h$ is invertible. Moreover,

$$\begin{aligned} &\left((I + ik\Lambda_s\mathcal{L}_h^s)^{-1}\right)_{m,l} = 0, && m > l, \\ &(-ikL_h)^{l-m}\,(I + ik\lambda_s L_h)^{-(l-m+1)}, && 1 \le m \le l \le i_s. \end{aligned} \tag{3.2}$$

Set $g(z) = (kz)^{l-m+\theta}\,(1 + ik\lambda_s z)^{-(l-m+1)}$. Then obviously $g(z)$ is continuous everywhere except at $z = -1/(ik\lambda_s) \notin R$. And also we can show that there exists a constant c independent of k such that

$$\sup_{z \in \sigma(L_h)} |g(z)| \le c.$$

By a spectral argument, it now follows from (3.2) that $\|(k\mathcal{L}_h^s)^{\theta}\,(I + ik\Lambda_s\mathcal{L}_h^s)^{-1}\| \le c$. This gives (3.1).

Now, sufficiently accurate starting approximations are assumed given and for $\nu - 1 \le n \le N-1$, an error equation relating $U_h^n - w^n$ to $U_h^{n+1} - w^{n+1}$ is presented. For the sequel, we make the following definitions:

$$\begin{aligned} &\xi^n \equiv U_h^n - w^n, \quad \eta^n \equiv u^n - w^n, \quad f^n \equiv f\left(x, t^n, u^n\right), \\ &\overline{u}^n \equiv \sum_{l=0}^{v} A^l e \partial_t^l u^n k^l, \quad \varepsilon_j^n f \equiv \sum_{m=0}^{\nu-1} \alpha_{j,m} f^{n-m}, \\ &f_h^n \equiv f\left(x, t^n, U_h^n\right), \quad \mathcal{L} \equiv \operatorname*{diag}_{q\times q}\{L\}, \quad \mathcal{P}_E \equiv \operatorname*{diag}_{q\times q}\{P_E\}, \\ r(ikL_h) &\equiv I - ikb^T\mathcal{L}_h(I + ikA\mathcal{L}_h)^{-1}\,e. \end{aligned}$$

After some calculations, the following error equation is obtained:

$$\begin{aligned} \xi^{n+1} &= r(ikL_h)\,\xi^n + ikb^T\mathcal{L}_h[I + ikA\mathcal{L}_h]^{-1}\,\mathcal{P}_0\{\overline{u}^n - eu^n + ikA\mathcal{L}\overline{u}^n - kA\varepsilon^n f\} \\ &\quad + ikb^T\mathcal{L}_h[I + ikA\mathcal{L}_h]^{-1}\,(\mathcal{P}_E - \mathcal{P}_0)\,(\overline{u}^n - eu^n) \\ &\quad + (P_0 - P_E)\left(u^{n+1} - u^n\right) \\ &\quad - P_0\left\{u^{n+1} - u^n + kb^T i\mathcal{L}\overline{u}^n - kb^T\varepsilon^n f\right\} \\ &\quad + kb^T[I + ikA\mathcal{L}_h]^{-1}\,\mathcal{P}_0[\varepsilon^n f_h - \varepsilon^n f] \\ &= r(ikL_h)\,\xi^n + \sum_{l=1}^{4}\Psi_l^n + \Phi^n, \qquad \nu - 1 \le n \le N-1. \end{aligned} \tag{3.3}$$

We begin by establishing a stability result for the operator $r(ikL_h)$.

PROPOSITION 3.1. *If the rational function* (2.13) *satisfies* (2.14), *then*

$$\|r(ikL_h)\| \le 1, \qquad \forall \chi \in S_h, \tag{3.4}$$

where $\|\cdot\|$ *also denotes the operator norm on* S_h.

PROOF. Since $L_h : S_h \to S_h$ is self-adjoint, it is easy to see that

$$\|r(ikL_h)\| = \max_{\lambda\in\sigma(L_h)} |r(ik\lambda)|.$$

Equation (3.4) now follows.

REMARK. In the special case of the Backward Euler scheme, $q = 1$, $(A)_{11} = b_1 = \tau_1 = 1$, we have $r(z) = 1/(z+1)$. It is not difficult to show that we can obtain the following stronger version of (3.4)

$$\|r(ikL_h)\| \le (1+\tilde{c})$$

for some constant $\tilde{c} < 0$. As a consequence, it can be shown that if the constant $C(\rho, u)$ in (2.16) is sufficiently small, then the error estimates are independent of t. However, the fact that $r(z)$ must be a good approximation to e^{iy}, $y \ge 0$, y small, restricts $r(z)$ to first order accuracy.

Next, the order of consistency is established in the following.

PROPOSITION 3.2. *The terms* $(\Psi_l^n)_{l=1}^4$ *of* (3.3) *satisfy*

$$\sum_{l=1}^{4} \|\Psi_l^n\| \le Ck(h^r + k^\nu)\left\{\left\|\partial_t^{\nu+1}u\right\|_{0,\infty} + \|\partial_t^\nu u\|_{2,\infty} + \|\partial_t u\|_{r,\infty}\right\}. \tag{3.5}$$

Also, if $[U_h^{n-m}]_{m=0}^{\nu-1}$ *are given and satisfy*

$$\max_{0\le m\le \nu-1} \left\|U_h^{n-m} - u^{n-m}\right\|_{L^\infty} \le \rho, \tag{3.6}$$

then Φ^n *of* (3.3) *satisfies*

$$\|\Phi^n\| \le Ckh^r\|u\|_{r,\infty} + CC(\rho,u)\,k\sum_{m=0}^{\nu-1}\left\|\xi^{n-m}\right\|. \tag{3.7}$$

PROOF. The terms of (3.3) are considered in the order in which they appear. Since for $0 \le 1 \le \nu$, $\partial_t^1 u \in H^2 \cap H_0^1$, by (1.1)

$$\begin{aligned}\overline{u}^n - eu^n + ikA\mathcal{L}u^n &= \sum_{l=1}^{\nu} A^1 e\,\partial_t^1 u^n k^l + \sum_{l=0}^{\nu} A^{l+1}e\left[iL\,\partial_t^l a\overline{u}^n\right]\,k^{l+1}\\ &= -A^{\nu+1}e\,\partial_t^{\nu+1}u^n k^{\nu+1} + kA\sum_{l=0}^{\nu} A^1 e\,\partial_t^l f^n k^l.\end{aligned}$$

By (2.17),

$$\varepsilon^n f = \sum_{l=0}^{\nu-1} A^l e\,\partial_t^l f^n k^l + E, \tag{3.8}$$

where E has components

$$E_j = \frac{1}{(\nu-1)!}\sum_{m=0}^{\nu-1}\alpha_{j,m}\int_{t^m}^{t^{n-m}} (t^{n-m}-t)^{\nu-1}\,\partial_t^\nu f(x,t,u(x,t))\,dt.$$

Now from (3.1) and (1.1), it follows that

$$\begin{aligned}\|\Psi_1^n\| &\le ck^{\nu+1}\left\{\left\|\partial_t^{\nu+1}u\right\|_{0,\infty} + \|\partial_t^\nu f\|_{0,\infty}\right\}\\ &\le ck^{\nu+1}\left\{\left\|\partial_t^{\nu+1}u\right\|_{0,\infty} + \|\partial_t^\nu u\|_{2,\infty}\right\}.\end{aligned} \tag{3.9}$$

Next, as with (2.17), the constants $[\beta_{j,m}]_{1\le j\le q}^{0\le m\le \nu}$ are well-defined by

$$\sum_{m=0}^{\nu} \beta_{j,m} m^l = l! \nu^l \hat{e}_j^T A^l e (1-\delta_{l0}), \qquad \begin{array}{l} 0 \le l \le \nu, \\ 1 \le j \le q. (m^l \mid_{m=l=0} = 1), \end{array}$$

where δ_{ij} is the Kronecker delta. Hence, define the extrapolation operator $\mathcal{X}^n$ to have components

$$\mathcal{X}_j^n \equiv \sum_{m=0}^{\nu} \beta_{j,m} u\left(t^n + \frac{mk}{\nu}\right), \qquad 1 \le j \le q,$$

so that for $0 \le p \le \nu$, with ill-defined sums understood to be zero,

$$\mathcal{X}^n u = \sum_{l=1}^{p} A^l e\, \partial_t^l u^n k^l + F^p,$$

where F^p has components

$$F_j^p = \frac{1}{p!} \sum_{m=0}^{\nu} \beta_{j,m} \int_{t^n}^{t^n+(mk/\nu)} \left(t^n + \frac{mk}{\nu} - t\right)^p \partial_t^{p+1} u(t)\, dt.$$

Now note that Ψ_2^n is given by:

$$\begin{aligned} \Psi_2^n &= ikb^T \left[I + ikA\mathcal{L}_h\right]^{-1} \mathcal{P}_0 \mathcal{L} \left[\overline{u}^n - eu^n - \mathcal{X}^n u\right] \\ &\quad - ikb^T \mathcal{L}_h \left[I + ikA\mathcal{L}_h\right]^{-1} \left\{\mathcal{P}_0 \left[\overline{u}^n - eu^n - \mathcal{X}^n u\right] + \left[\mathcal{P}_0 - \mathcal{P}_E\right] \mathcal{X}^n u\right\}. \end{aligned}$$

From (3.1), (2.5) and (2.6), it follows that

$$\begin{aligned} \|\Psi_2^n\| &\le ck \left\|\mathcal{L}\left[A^\nu e\, \partial_t^\nu u^n k^\nu - F^{\nu-1}\right]\right\| + c\|F^\nu\| + c\left\|\left[\mathcal{P}_0 - \mathcal{P}_E\right] F^0\right\| \\ &\le ck\left(k^\nu + h^r\right)\left\{\|\partial_t^\nu u\|_{2,\infty} + \left\|\partial_t^{\nu+1} u\right\|_{0,\infty} + \|\partial_t u\|_{r,\infty}\right\}. \end{aligned} \tag{3.10}$$

Now, since

$$\Psi_3^n = \int_{t^n}^{t^{n+1}} (P_0 - P_E)\, \partial_t u(t)\, dt,$$

from (2.5) and (2.6), it follows that

$$\|\Psi_3^n\| \le ckh^r \|\partial_t u\|_{r,\infty}. \tag{3.11}$$

Next, using (1.1), (3.8) and (2.12), the following is obtained.

$$\begin{aligned} \Psi_4^n &= -P_0 \left\{ G + \sum_{l=0}^{\nu-1} \partial_t^{l+1} u^n \frac{k^{l+1}}{(l+1)!} + \sum_{l=0}^{\nu} b^T A^l e \left[iL\, \partial_t^l u^n\right] k^{l+1} \right. \\ &\qquad \left. - \sum_{l=0}^{\nu-1} b^T A^l e\, \partial_t^l f^n k^{l+1} - kb^T E \right\} \\ &= -P_0 \left\{ G + b^T A^\nu e \left[iL\, \partial_t^\nu u^n k^{\nu+1}\right] - kb^T E \right\}, \end{aligned}$$

where

$$G = \frac{1}{\nu!} \int_{t^n}^{t^{n+1}} (t^{n+1} - t)^\nu\, \partial_t^{\nu+1} u(t)\, dt.$$

Then from (1.1)

$$\begin{aligned} \|\Psi_4^n\| &\le ck^{\nu+1} \left\{ \left\|\partial_t^{\nu+1} u\right\|_{0,\infty} + \|\partial_t^\nu u\|_{2,\infty} + \|\partial_t^\nu f\|_{0,\infty} \right\} \\ &\le ck^{\nu+1} \left\{ \left\|\partial_t^{\nu+1} u\right\|_{0,\infty} + \|\partial_t^\nu u\|_{2,\infty} \right\}. \end{aligned} \tag{3.12}$$

Now, (3.5) follows after combining (3.9)–(3.12). Finally, because of (3.6), (2.16) and (3.1)

$$\begin{aligned}\|\Phi^n\| &\le ck \sum_{m=0}^{\nu-1} \|f_h^{n-m} - f^{n-m}\| \\ &\le cC(\rho, u)\, k \sum_{m=0}^{\nu-1} \|\xi^{n-m} - \eta^{n-m}\|\end{aligned}$$

and (3.7) follows from (2.5).

Now set

$$N(u) \equiv \|u\|_{r,\infty} + \|\partial_t u\|_{r,\infty} + \sum_{l=1}^{\nu} \left\|\partial_t^l u\right\|_{2,\infty} + \left\|\partial_t^{\nu+1} u\right\|_{0,\infty}.$$

Then (2.24) is finally established in the following.

THEOREM 3.1. *Assume that* (2.14) *and* (2.15) *hold. Suppose* $[U_h^m]_{m=0}^{\nu-1}$ *are given satisfying*

$$\max_{0\le m\le \nu-1} \|U_h^m - u^m\| \le c(h^r + k^\nu). \tag{3.13}$$

Then, provided $h^{-d/2}(h^r + k^\nu) + r_0(h)$ *is sufficiently small,* $[U_h^n]_{n=\nu}^N$ *are well-defined by* (2.19) *and*

$$\max_{0\le n\le N} \|U_h^n - u^n\| \le c(u)(h^r + k^\nu). \tag{3.14}$$

PROOF. Set $\Theta(h,k) \equiv h^{-d/2}(h^r + k^\nu) + r_0(h)$. It is first established that for $\Theta(h,k)$ small enough

$$\max_{0\le m\le N} \|U_h^m - u^m\|_{L^\infty} \le \rho. \tag{3.15}$$

Note that by (2.4), (3.13) and (2.7), for $\Theta(h,k)$ small enough,

$$\begin{aligned}\|U_h^m - u^m\|_{L^\infty} &\le Ch^{-d/2}\|\xi^m\| + \|\eta^m\|_{L^\infty} \\ &\le Ch^{-d/2}(h^r + k^\nu) + r_0(h) \\ &\le c\Theta(h,k) \\ &\le \rho, \qquad 0 \le m \le \nu - 1.\end{aligned}$$

Now suppose that for some h, k, sufficiently small, there exists an $n = n(h,k)$ such that $\nu - 1 \le n \le N - 1$ and

$$\max_{0\le l\le n} \left\|U_h^l - u^l\right\|_{L^\infty} \le \rho. \tag{3.16}$$

Given (3.16), inequalities (3.4), (3.5) and (3.7) can be combined with the error equation (3.3) to obtain

$$\begin{aligned}\left\|\xi^{l+1}\right\| \le{}& (1 + \tilde{c}k) \left\|\xi^l\right\| + c_1 k\,(h^r + k^\nu)\, N(u) \\ &+ c_2 C(\rho, u)\, k \sum_{m=0}^{\nu-1} \left\|\xi^{l-m}\right\|, \qquad \nu - 1 \le l \le n\end{aligned} \tag{3.17}$$

for some constants $c_1, c_2 > 0$. It follows from a Gronwall type argument that

$$\left\|\xi^{n+1}\right\| \le \hat{c} \left\{ c_1\,(h^r + k^\nu)\, N(u) + c_2 C(\rho, u) \sum_{m=0}^{\nu-1} \|\xi^m\| \right\}, \tag{3.18}$$

where $\hat{c}$ depends exponentially on T and $C(\rho,u)$, unless $\tilde{c}$ is sufficiently negative so that $\tilde{c} < -c_2 C(\rho,u)\,\nu$ holds. Now by (2.4), (3.18), (3.13) and (2.7), for $\Theta(h,k)$ sufficiently small

$$\begin{aligned}\left\|U_h^{n+1} - u^{n+1}\right\|_{L^\infty} &\le ch^{-d/2} \left\|\xi^{n+1}\right\| + \left\|\eta^{n+1}\right\|_{L^\infty} \\ &\le c\Theta(h,k) \le \rho.\end{aligned}$$

By induction, we conclude that (3.15) holds. With this, we obtain (3.17) for $l = \nu - 1, \dots, n + 1$. Repeating this argument, we obtain (3.14).

4. THE NLS EQUATION WITH PERIODIC B.C.

In this section, we indicate how the results obtained earlier can be extended to handle the NLS equation with periodic boundary conditions. Aside from the fact that such B.C. are of practical interest, they can also be used to numerically simulate the solutions of the NLS equation posed on the entire real line provided such solutions decay sufficiently fast.

Hence, let Ω now denote a d-dimensional rectangle, and assume that the data u^0 is periodic over Ω and that (1.1) has a smooth periodic solution. In this case, H^r_{per} will denote the subspace of H^r consisting of periodic functions. Also, S_h will denote a subspace of H^1_{per} endowed with the approximation property

$$\inf_{\chi\in S_h}\left(\|v-\chi\|+h\|v-\chi\|_1\right)\le ch^s\|v\|_s,\qquad v\in H^s_{\text{per}},\quad 1\le s\le r. \tag{4.1}$$

The main difficulty here is that the bilinear form $(\nabla\cdot,\nabla\cdot): S_h\times S_h\to R$ is not coercive. Hence, define $T_h: L^2\to S_h$ such that

$$(\nabla T_h w,\nabla\chi)+(T_h w,\chi)=(w,\chi),\qquad \forall\chi\in S_h;$$

then T_h is positive definite on S_h. Also, we can define the inverse of T_h on S_h as $T_h^{-1}=-\Delta_h+I$, where the discrete Laplacian $\Delta_h: S_h\to S_h$ is now given by

$$(\Delta_h w,\chi)=-(\nabla w,\nabla\chi),\qquad \forall\chi\in S_h.$$

Define an elliptic projection operator $P_E: H^1_{\text{per}}\to S_h$ such that

$$(\nabla P_E v,\ \nabla\chi)+(P_E v,\chi)=(\nabla v,\nabla\chi)+(v,\chi),\qquad \forall\chi\in S_h. \tag{4.2}$$

Then it is well known that (2.5) holds, i.e.,

$$\|(I-P_E)\,v\|\le Ch^s\|v\|_s,\qquad \forall v\in H^s_{\text{per}},\quad 2\le s\le r.$$

And we have obviously the following:

(i) $((-\Delta_h+I)\,v,v)$ is real, $\forall v\in S_h$;
(ii) $P_E=T_h(L+I)$ and $((-\Delta_h+I)\,v,v)\ge c\|v\|_1^2$, $\forall v\in S_h$, for some constant c;
(iii) $P_0=(-\Delta_h+I)\,T_h$.

For the periodic boundary-value problem, we can easily prove that all the requirements and theorems in Sections 2 and 3 can be established by replacing Lu by $Lu+u$, $f(x,t,u)$ by $i\beta u+f(x,t,u)$, L_h by $(-\Delta_h+I)$ and $-i$ (or i) by $-\beta i$ (or βi).

5. COMPUTATIONAL ASPECTS

In this section, we describe results of numerical experiments designed to measure the performance of the numerical methods introduced earlier.

Consider the following problem.

$$\begin{aligned} u_t &= -i\,\frac{1}{40}\,u_{xx}-128000i\,|u|^2\,u, && (x,t)\in R\times[0,T],\\ u(x,0) &= \frac{1}{40}\,e^{-i(80x+(\pi/2))}\operatorname{sech}(40(x-0.5)), && x\in R, \end{aligned} \tag{5.1a}$$

whose solution is

$$u(x,t)=\frac{1}{40}\,e^{-i(80(x-4t)+200t+(\pi/2))}\operatorname{sech}(40(x-4t-0.5)). \tag{5.1b}$$

The modulus of the initial condition is a solitary wave of amplitude $1/40$, centered at $x = 0.5$ and of support essentially in $[0.1, 0.9]$. Although (5.1b) is a solution to the pure initial-value problem (5.1a) on the whole real line, it may be considered as a good approximation to the solution corresponding to the periodic boundary conditions since the tails of the solution decay exponentially. For $t > 0$, this moves to the right without change of form with speed 4 and has completed $1/2$ revolution at $t = 0.125$.

It is straightforward to see that the L^2 norm of the solution $u(.,t) = u(t)$ of (5.1) is an invariant of the equation, i.e., that

$$I_1(t) \equiv \|u(t)\| = \|u(0)\|. \tag{5.2}$$

To see this, multiply the first equation of (5.1a) by $\overline{u}$, integrate over x and take real parts. In addition, we obtain the second invariant,

$$\begin{aligned} I_2(t) &\equiv \frac{1}{40}\,\|u_x(\cdot,t)\|^2 - 64000\|u(\cdot,t)\|_{L^4}^4 \\ &= \frac{1}{40}\,\|u_x(\cdot,0)\|^2 - 64000\|u(\cdot,0)\|_{L^4}^4, \end{aligned} \tag{5.3}$$

which is obtained by multiplying the equation by $\overline{u}_t$, integrating and taking imaginary parts. We use the schemes (2.19) and (2.22) in their complex formulation, adapted of course to equation (5.1a) which has $-(1/40)\,u_{xx}$ instead of u_{xx}. As S_h we take the space of smooth periodic splines of order r (degree $r-1$) on a uniform mesh with mesh length h.

For the time stepping procedure, we use two or three stage Gauss Legendre method with constants a_{ij}, b_i, τ_i, $1 \le i,j \le q$, (where $q = 2$ or $q = 3$) given by the following.

$$\begin{array}{cc|c} \frac{1}{4} & \frac{1}{4}-\frac{1}{2\sqrt{3}} & \frac{1}{2}-\frac{1}{2\sqrt{3}} \\ \frac{1}{4}+\frac{1}{2\sqrt{3}} & \frac{1}{4} & \frac{1}{2}+\frac{1}{2\sqrt{3}} \\ \hline \frac{1}{2} & \frac{1}{2} & \end{array} \qquad \begin{array}{ccc|c} \frac{5}{36} & \frac{80-24\sqrt{15}}{360} & \frac{50-12\sqrt{15}}{360} & \frac{1}{2}-\frac{\sqrt{15}}{10} \\ \frac{50+15\sqrt{15}}{360} & \frac{2}{9} & \frac{50-15\sqrt{15}}{360} & \frac{1}{2} \\ \frac{50+12\sqrt{15}}{360} & \frac{80+24\sqrt{15}}{360} & \frac{5}{36} & \frac{1}{2}+\frac{\sqrt{15}}{10} \\ \hline \frac{5}{18} & \frac{8}{18} & \frac{5}{18} & \end{array}$$

The 2 stage and 3 stage Gauss-Legendre method satisfies (2.12) with $\nu = 4$ and 6, respectively. Since these two methods satisfy (2.14), the constant C in Theorem 3.1 depends exponentially on T as we mentioned above. For both methods, A can be transformed into $A = S^{-1}\Lambda S$ where Λ is a complex-valued diagonal matrix $\Lambda = \operatorname{diag}_{1\le i\le q}\{\lambda_i\}$. Then the linear system from (2.19) or (2.22) can be written as

$$[I + ik\Lambda L]\, S\Phi = S\Psi,$$

which decouples to equations of the form

$$[I + ik\lambda_i L]\,\phi_i = \Psi_i, \qquad i = 1,\dots,q \ \text{ (where } q = 2 \text{ or } 3). \tag{5.4}$$

All of the experiments reported in the sequel were performed in double precision using complex arithmetic on the SPARC station 1 (manufactured by the Sun Microsystems Inc.).

Next we report the outcome of a number of numerical experiments that were performed on (5.1a). First, the convergence rates of the scheme in the temporal variable were investigated for $r = 3, 4, 6$. The errors were measured both in the usual and normalized versions of the L^2-norm according to

$$E(t) = \|U^n - u(\cdot,t^n)\|, \quad N(t) = \frac{\|U^n - u(\cdot,t^n)\|}{\|u_0\|}, \qquad \text{if } t = nk, \quad n = 1,2,\dots.$$

The experimental determination of the temporal accuracy is a somewhat delicate matter because long runs with very small values of h are extremely expensive, both in terms of run time and storage. To avoid this, we used the following very efficient device introduced in [13]. For a fixed h, we make a reference calculation with a sufficiently small $k = k_{\rm ref}$. For the same value h, we then defined a modified error associated to values of k that are larger than $k_{\rm ref}$, namely,

$$E^*(t) = \|U^n(h,k) - U^m(h,k_{\rm ref})\|, \quad N^*(t) = \frac{\|U^n(h,k) - U^m(h,k_{\rm ref})\|}{\|u_0\|},$$

where $t = nk = mk_{\rm ref}$. Each of $E^*(t)$ and $N^*(t)$ can be considered as a pure temporal error because subtracting $U^m(h,k_{\rm ref})$ from $U^n(h,k)$ essentially cancels the spatial error inherent in the latter approximation.

The results of these comparisons are shown in Tables 1 and 2, which refer to splines of order 3, 4 and 6. The expected temporal rate of convergence, $\nu = 4, 6$, respectively, emerges clearly from these experiments for the 2 stage or the 3 stage Gauss Legendre method, respectively. Therefore, for the values k where the temporal rate of convergence is close to the theoretical value ν, the temporal error can be expressed as

$$E^*(t) = C_2 k^\nu \text{ and } N^*(t) = C_3 k^\nu.$$

For the 2 stage Gauss-Legendre method, from Table 1, $C_2 \cong 1.4 \times 10^8$ $C_3 \cong 2.7 \times 10^{10}$ emerge as values that fit the data independently of h and the order of splines used.

Table 1a. $T = 0.125$, $k_{\rm ref} = 1/5000$, $h^{-1} = 200$, $r = 4$.

N	h^{-1}/N	$E(t)$	$E^*(t)$	Rate
100	2	0.7826(−3)	0.7826(−3)	4.67
200	1	0.3074(−4)	0.3074(−4)	4.45
300	2/3	0.5056(−5)	0.5056(−5)	4.26
400	1/2	0.1486(−5)	0.1485(−5)	4.14
500	2/5	0.5906(−6)	0.5902(−6)	4.07
600	1/3	0.2816(−6)	0.2812(−6)	4.01
700	2/7	0.1516(−6)	0.1516(−6)	
5000	1/25	0.7796(−8)		

Table 1b. $T = 0.125$, $k_{\rm ref} = 1/7500$, $h^{-1} = 300$, $r = 3$.

N	h^{-1}/N	$E(t)$	$E^*(t)$	Rate
150	2	0.1168(−3)	0.1154(−3)	4.51
300	1	0.1068(−4)	0.5051(−5)	4.23
450	2/3	0.7520(−5)	0.9095(−6)	4.08
600	1/2	0.7016(−5)	0.2810(−6)	4.02
750	2/5	0.6872(−5)	0.1145(−6)	
7500	1/25	0.6766(−5)		

For the 3-stage Gauss-Legendre method, from Table 2, $C_2 \cong 3.1 \times 10^{13}$ $C_3 \cong 5.7 \times 10^{15}$ fit the data again independently of h and the order of splines used.

The constants C_2, C_3 are rather large because the temporal rate depends on $\|\partial_t^{\nu+1} u\|_{0,\infty} \cong (160)^{\nu+1}$ and $\|\partial_t^\nu u\|_{2,\infty} \cong (160)^\nu (80)^2$.

From Tables 1 and 2, we can conclude that our computational implementation conforms to the results of Sections 3 and 4 very well.

The next set of experiments reported here feature computing the approximate solution of (5.1a) up to $T = 1.0$ in order to study the behavior of various kinds of errors over a longer temporal interval. In addition to the L_2-error $E(t)$, we also monitored the L_2-error of modulus, the L_2-based shape error and the phase error.

Table 2a. $T = 0.125$, $k_{\text{ref}} = 1/7000$, $h^{-1} = 150$, $r = 6$.

N	h^{-1}/N	$E(t)$	$E^*(t)$	Rate
300	1/2	0.3946(−6)	0.3949(−6)	7.54
500	3/10	0.6603(−7)	0.8376(−8)	6.25
600	1/4	0.6607(−7)	0.2679(−8)	6.17
700	3/14	0.6620(−7)	0.1035(−8)	6.12
800	3/16	0.6627(−7)	0.4572(−9)	6.08
900	1/6	0.6630(−7)	0.2234(−9)	6.05
1000	3/20	0.6631(−7)	0.1181(−9)	
7000	3/140	0.6632(−7)		

Table 2b. $T = 0.125$, $k_{\text{ref}} = 1/6000$, $h^{-1} = 100$, $r = 4$.

N	h^{-1}/N	$N(t)$	$N^*(t)$	Rate
200	1/2	0.1288(−1)	0.4523(−2)	11.80
300	1/3	0.1206(−1)	0.3810(−4)	6.41
400	1/4	0.1207(−1)	0.6019(−5)	6.29
500	1/5	0.1207(−1)	0.1478(−5)	6.20
600	1/6	0.1208(−1)	0.4773(−6)	6.13
700	1/7	0.1208(−1)	0.1855(−6)	6.09
800	1/8	0.1208(−1)	0.8226(−7)	6.06
900	1/9	0.1208(−1)	0.4027(−7)	
6000	1/60	0.1208(−1)		

The L_2-error of modulus $M(t)$ at t is defined by

$$M(t) = \left[\int_0^1 \left(|u(x,t)| - |U^n(x)|\right)^2 dx\right]^{1/2}, \qquad \text{where } nk = t.$$

The shape error S^n is defined for each time step $n = 0, 1, 2, \ldots, J$ as follows.

Fix n and consider the quantity

$$\mathcal{E}(\tau) = \left[\int_0^1 \left(|u(x,\tau)| - |U^n(x)|\right)^2 dx\right]^{1/2},$$

where $u(x,\tau)$ is given in (5.1b) and U^n is the computed solution at the n^{th} time step. Let $\tau^* = \tau^*(n)$ denote the value of τ near nk where $\mathcal{E}(\tau)$ takes its minimum value. If $|U^n|$ resembles a solitary wave in shape, it follows that τ^* is well-defined. Then S^n measures how far the computed solution differs from the original solution as regards to its shape.

The phase error p^n at any time step n with $0 \le n \le J$ is defined to be $|nk - \tau^*(n)|$. This quantity measures the error in the position at which the wave is located.

In Table 3, errors are shown at times $t = 0.2, 0.4, 0.6, 0.8$ and 1.0 for the 2 stage Gauss-Legendre method with parameters $r = 4$, $h = 1/100$ and $k = 1/1500$ on the temporal interval [0,1].

Table 3.

t	$E(t)$	Modulus Error	Shape Error	Phase Error
0.2	0.1391(−3)	0.1217(−3)	0.1515(−3)	0.2340(−3)
0.4	0.3925(−3)	0.3911(−3)	0.1597(−4)	0.7573(−3)
0.6	0.8365(−3)	0.8126(−3)	0.2000(−4)	0.1576(−2)
0.8	0.1477(−2)	0.1381(−2)	0.2632(−4)	0.2694(−2)
1.0	0.2299(−2)	0.2084(−2)	0.4369(−4)	0.4122(−2)

In Figure 1, we show $E(t)$ and the phase error as functions of time for the data in Table 3. As we expected, $E(t)$ and the phase error exhibit exponential growth approximately. And $M(t)$ exhibits similar to that of $E(t)$, but the shape error stays small.

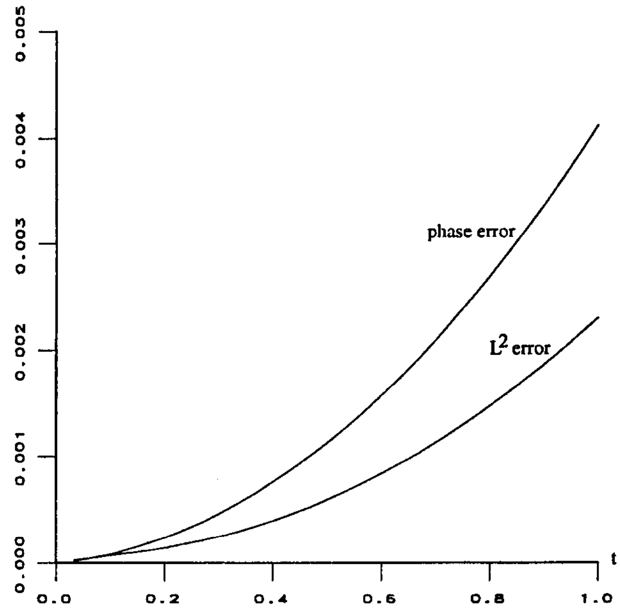

Figure 1. 2-stage G-L method, $r = 4$, $h = 1/100$, $k = 1/1500$.

We also investigated the effect of choosing h and especially k sufficiently small on the growth of the above quantities as a function of t. For the 2-stage Gauss Legendre method we took $r = 4$, $h = 1/150$ and $k = 1/8000$. Indeed, as Table 4 and the corresponding Figure 2 indicate, $E(t)$, $M(t)$ and the phase error grow linearly rather than exponentially.

Table 4.

t	$E(t)$	Modulus Error	Shape Error	Phase Error
0.2	0.5724(−5)	0.2246(−5)	0.1197(−5)	0.3667(−5)
0.4	0.1136(−4)	0.4015(−5)	0.1191(−5)	0.7417(−5)
0.6	0.1681(−4)	0.5928(−5)	0.1118(−5)	0.1125(−4)
0.8	0.2227(−4)	0.7894(−5)	0.1138(−5)	0.1517(−4)
1.0	0.2785(−4)	0.9949(−5)	0.1199(−5)	0.1917(−4)

Attention is now turned to the conservation of two invariants defined by (5.2) and (5.3). We computed with periodic cubic splines and evaluated the integrals in the inner products using the 7-point Gauss rule on each subinterval of the spatial discretization so that the nonlinear term is computed exactly.

In Table 5, we show I_1 and I_2 at $t = 0, 0.125, 0.25, 0.375$ and 0.5 with values of h equal to $1/100$, $1/150$ and N equal to 600 and 900. This table indicates that the code preserves these two invariants well.

Finally, we give some computational results which show that there is no effect when approximating the pure initial value problem (5.1a) by a periodic boundary value problem.

To apply the spatial and temporal discretization introduced in Section 2 with the pure initial value problem at $T = 0.125$, we need to choose the space interval $[0.0, 1.5]$ so that the support of $u(x,t)$, $0 \le t \le T = 0.125$, stays inside $[0.0, 1.5]$. We can take S_h as, for example, the space of splines of order r with a 0-boundary condition on a uniform mesh with mesh length h.

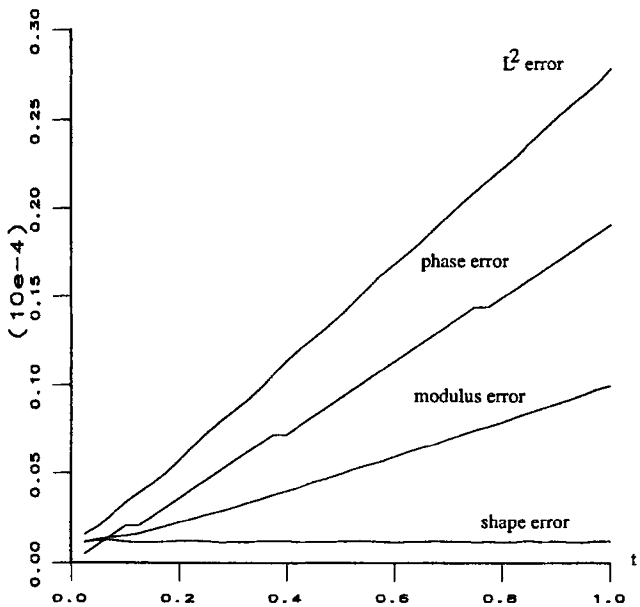

Figure 2. 2-stage G-L method, $r = 4$, $h = 1/150$, $k = 1/8000$.

Table 5.

	$h = 1/100$	$N = 600$	$h = 1/150$	$N = 600$
t	$I_1(t)$	$I_2(t)$	$I_1(t)$	$I_2(t)$
0.0	0.00559	0.00229	0.0055902	0.0022917
0.125	0.00560	0.00231	0.0055913	0.0022944
0.25	0.00561	0.00233	0.0055924	0.0022971
0.375	0.00561	0.00235	0.0055935	0.0022997
0.5	0.00562	0.00237	0.0055946	0.0023024

Table 6.

Periodic B.C.			Dirichlet B.C.		
h	N	$E(t)$	h	N	$E(t)$
1/100	100	0.7468(−3)	1.5/150	100	0.7468(−3)
1/200	200	0.3092(−4)	1.5/300	200	0.3092(−4)
1/300	300	0.5079(−5)	1.5/450	300	0.5079(−5)
1/400	400	0.1490(−5)	1.5/600	400	0.1490(−5)

As shown in Table 6, the periodic B.C. approach produces errors comparable to the 0 Dirichlet B.C. ones while the storage and CPU time requirements of the latter are about $1 + (\text{speed})T$ those of the former.

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